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OCO (Orbiting Carbon Observatory) – 2

Science Validation Plan

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Jet Propulsion Laboratory
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ORBITING CARBON OBSERVATORY (OCO) -2

SCIENCE VALIDATION PLAN

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1. The OCO-2 Science Validation Strategy

The primary responsibility of the OCO-2 Science Validation system is to provide ground truth for the column averaged CO_2 dry air mole fraction (X_{CO2}) data products retrieved from space-based measurements of sunlight reflected from the Earth's surface. The ability to "Compare space-based and ground-based X_{CO2} retrievals from soundings collected during over-flights of ≥ 3 primary ground validation sites at least once each season to identify and correct global-scale systematic biases in the space-based X_{CO2} product and to demonstrate a precision of ≤ 0.5% for collections of ≥100 cloud-free soundings" [**L1-Req-9**[1]] defines the highest level validation requirement for the OCO-2 Project. It is critical that OCO-2 deliver X_{CO2} data without significant uncharacterized random errors and systematic biases since these will induce spurious errors or incorrect carbon flux estimates when ingested into models with other atmospheric CO_2 data. Another major challenge is that the Science Validation system must link OCO-2 X_{CO2} data to the point measurements from the National Oceanic and Atmospheric Administration (NOAA) in situ CO_2 data record, the World Meteorological Organization (WMO) Standard which serves as the de facto foundation for all current and future scientific investigations of atmospheric CO_2 and the global carbon cycle.

1.1 Science Validation Program Overview

The OCO-2 Validation program links in situ CO_2 point measurements calibrated to the WMO reference standards to OCO-2 regional-scale X_{CO2} [**L3-Val-29**]. The network of calibrated ground-based solar-viewing Fourier transform spectrometers (FTSs) in the Total Carbon Column Observing Network (TCCON), provides the transfer standard between the OCO-2 space-based X_{CO2} and the WMO CO_2 standard. FTS X_{CO2} will be calibrated to the WMO CO_2 standard via over-flights of the FTS validation sites by aircraft or balloons carrying instruments that acquire in situ CO_2 measurements tied to the WMO standard.

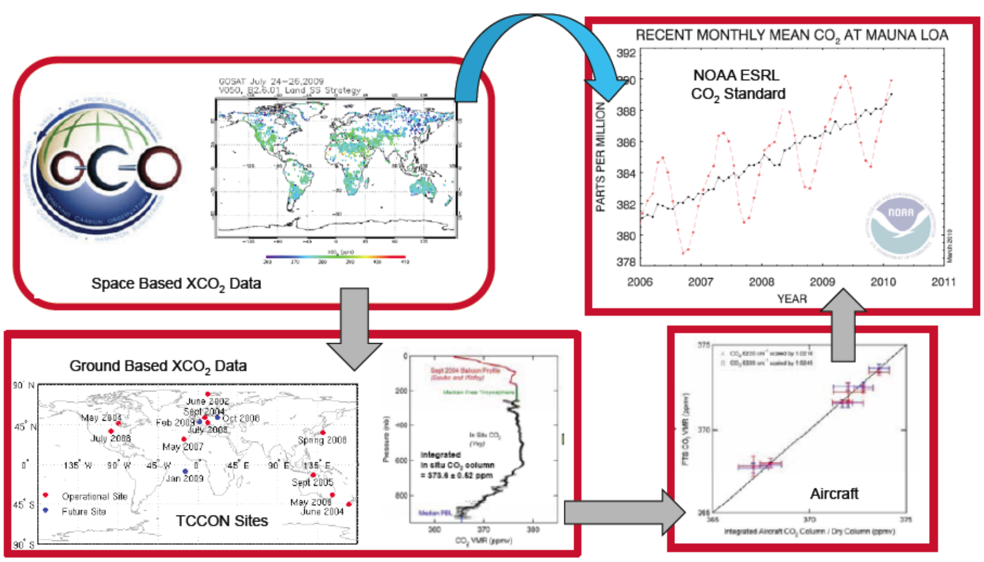

Figure 1-1 Validation strategy to link OCO-2 Regional X_{CO2} to the WMO CO_2 Reference Standard, satisfying Level 1 Science Measurement Validation Requirements.

[1] Throughout this document, references to OCO-2 requirements are indicated in blue text.

The on-orbit Validation strategy includes an Observatory point-and-stare Target mode, in which the Observatory acquires thousands of observations at a fixed surface site as it flies over the selected location. Target mode data acquired over FTS validation sites and the resulting analyses, including FTS X_{CO2}/OCO-2 X_{CO2} regressions provide powerful tests of the OCO-2 measurement/retrieval system.

We note the intrinsic link between X_{CO2} data products and the Full Physics retrieval algorithm. The validation of X_{CO2} allows for a quantification of inadequacies in the physical approximations of the retrieval algorithm, and diagnostic outputs of the retrieval algorithm help the validation team assess the impacts of non-X_{CO2} geophysical variables, instrument performance, radiometric and spectral calibration, etc. on the accuracy of the X_{CO2} product. The Full Physics algorithm has been designed to retrieve X_{CO2} from both space-based and ground-based FTS spectra to minimize potential biases and facilitate the direct quantitative comparison of OCO-2 X_{CO2} and FTS X_{CO2}.

The Validation system thus integrates the following elements:

- FTS validation network establishment, operations, and observations
- Target Mode planning and observations
- Ancillary geophysical data acquisition
- Diagnostic outputs from the Full Physics retrieval algorithm

1.2 Key Validation Related Publications and Documents

This document is based largely on the Validation Plan written for the OCO instrument and mission. In the time since that document was released, several key papers describing the TCCON network/data and validation studies using those data have been published. A list of the documents is provided below.

- Wunch et al., Calibration of the Total Carbon Column Observing Network using aircraft profile data, *Atmospheric Measurement Techniques, 3,* 1351–1362, doi:10.5194/amt-3-1351-2010, http://www.atmos-meas-tech.net/3/1351/2010/, 2010.

- Wunch et al., The Total Carbon Column Observing Network, Phil. Trans. R. Soc. A, 369, 2087–2112, doi:10.1098/rsta.2010.0240, 2011a.

- Wunch et al., A method for evaluating bias in global measurements of CO_2 total columns from Space, *Atmos. Chem. Phys. Discuss., 11,* 20899-20946, 2011b.

- Keppel-Aleks et al., Sources of variations in total column carbon dioxide, *Atmospheric Chemistry and Physics, 11,* 3581–3593, doi:10.5194/acp-11-3581-2011, http://www.atmos-chem-phys.net/11/3581/2011/, 2011.

- Wofsy et al., HIAPER Pole-to-Pole Observations (HIPPO): Fine grained, global scale measurements of climatically important atmospheric gases and aerosols, *Phil. Trans. R. Soc. A,* **369**, 2073–2086, doi:10.1098/rsta.2010.0313, 2011.

- Washenfelder et al., Carbon dioxide column abundances at the Wisconsin Tall Tower site, *J. Geophys. Res, 111,* D22305, doi:10.1029/2006JD007154, 2006.

- Deutscher et al., Total column CO_2 measurements at Darwin, Australia - site description and calibration against in situ aircraft profiles, *Atmos. Meas. Tech., 3*, 947–958, doi:10.5194/amt-3-947-2010, 2010.
- Messerschmidt et al., Calibration of TCCON column-averaged CO_2: the first aircraft campaign over European TCCON sites, *Atmos. Chem. Phys. Discuss., 11,* 14 541–14 582, doi:10.5194/acpd-11-14541-2011, 2011.

These papers provide the basis for validating the OCO-2 data. Wunch et al. [2010] describes the methodology and status of the calibration of the TCCON network and its connection to the WMO standard [**L3-Val-26, L3-Val-29**]. Wunch et al. [2011a] is a description of the TCCON network. Wunch et al. [2011b] discusses the methodology for estimating biases and systematic errors in space based retrievals of X_{CO2} using data from the Japanese GOSAT satellite instrument with the TCCON data. The methods used in Wunch et al. [2011b] will be the primary analyses that will be performed by the OCO-2 validation team. Keppel-Aleks et al. [2011] describe the correlation between free tropospheric temperature and X_{CO2}, this correlation is used in the analysis of Wunch et al. [2011b]. Wofsy et al. [2011] is an overview of the HIAPER Pole-to-Pole Observations (HIPPO) aircraft campaign. Data from HIPPO and other aircraft campaigns are vital to calibrating the TCCON data and tying satellite observations of X_{CO2} to the WMO standard. Washenfelder et al. [2006] provides a description of the TCCON instruments and properties of the measurements that are vital to OCO-2 meeting its validation requirements [**L3-Val-25, L3-Val-27**]. Lastly the TCCON Wiki page (https://tccon-wiki.caltech.edu/) provides the most up-to-date information on the TCCON network and instrument status.

1.3 OCO-2 Mission Requirements Related to Validation

Many of the OCO-2 mission science requirements are directly related to work that will be performed as part of the Validation program. These requirements are listed in this section and references to specific requirements will be provided throughout this document to highlight validation work that specifically addresses them.

Level 1 Requirements Related to Validation Activities

L1-REQ-7: Retrieve estimates of the column-averaged CO_2 dry air mole fraction (X_{CO2}) on regional scales (≥1000 km) from space-based measurements of the absorption of reflected sunlight by atmospheric CO_2 and O_2, collected in cloud-free scenes over ≥ 80% of the range of latitudes on the sunlit hemisphere at monthly intervals for 2 years.

L1-REQ-9: Compare space-based and ground-based X_{CO2} retrievals from soundings collected during over-flights of ≥ 3 primary ground validation sites at least once each season to identify and correct global-scale systematic biases in the space-based X_{CO2} product and to demonstrate a precision of ≤ 0.3% for collections of ≥100 cloud-free soundings.

Level 3 Science Requirements Related to Validation Activities

L3-Val-23: The OCO-2 space-based retrievals shall be validated using observations from at least 7 FTS validation sites, selected to span a range of latitudes and longitudes.

L3-Val-24: Primary ground validation sites shall include:

- Park Falls, WI
- Lamont, OK
- Lauder, NZ
- Darwin, Australia

L3-Val-25: At primary validation sites, the ground-based FTS systems used for OCO-2 validation shall simultaneously observe near infrared CO_2 and O_2 absorptions in the same spectral regions that are used for the OCO-2 flight instrument soundings.

L3-Val-26: The NOAA ESRL CO_2 standard shall be used for calibration of the ground-based FTS systems.

L3-Val-27: The ground-based FTS instruments used for OCO-2 validation shall be operated with a HCl cell installed during data acquisition.

L3-Val-28: Each primary FTS validation site shall be calibrated by aircraft in situ CO_2 observations from the boundary layer to the middle troposphere (≥10 km altitude) at least once prior to the end of the OCO-2 science mission.

L3-Val-29: The aircraft in situ observations of CO_2 shall be traceable to the NOAA ESRL standard.

L3-Val-30: At primary validation sites, the ground-based FTS instruments shall have a clear-sky rms calibrated X_{CO2} accuracy of <=0.3% for soundings taken within +/- 30 minutes of a targeted over-flight.

L3-Val-31: The validation team shall demonstrate validation of the OCO-2 space-based surface pressure retrievals over oceans and topographically flat regions to an accuracy ≤ 1 mbar.

L3-Val-32: During pre-launch testing of the flight instrument, simultaneous data will be collected along the same atmospheric optical path by a co-located, solar-looking FTS.

L3-Val-33: During pre-launch testing of the flight instrument, the spectra simultaneously acquired from the collocated flight instrument and ground-based FTS shall be analyzed using the same retrieval algorithm to define the level of agreement between measurements of X_{CO2} from the two systems.

L3-Val-34: The validation team shall quantify the bias in space-based X_{CO2} retrievals as a function of geophysical and observation variables, including humidity, temperature, solar zenith angle, and aerosol optical depth.

L3-Val-35: The validation team shall compare X_{CO2} retrievals from OCO-2 Target Observations with coincident X_{CO2} retrievals from the targeted FTS validation site.

L3-Val-36: The validation team shall demonstrate comparison of space-based X_{CO2} retrievals with coincident X_{CO2} retrievals from FTS validation sites.

L3-Val-37: The validation team shall quantify biases in the exploratory X_{CO2} data product within 90 days of the end of IOC.

L3-Val-38: The validation team shall request ≥9 target opportunities for each primary validation site during the first year of science operations.

L3-Val-39: To enable a planned Target Observation, the validation team shall submit a CAR to the MOC at least two hours prior to the uplink pass preceding the Target Observation.

L3-Val-40: During the OCO-2 nominal mission, primary and supporting ground validation sites shall deliver all surface pressure measurements, X_{CO2} retrievals, averaging kernels, and a priori information to a Caltech TCCON repository.

L3-Val-41: During the OCO-2 nominal mission, primary ground validation sites shall deliver all collected spectra and runlogs to a Caltech TCCON repository.

L3-Val-42: During the OCO-2 nominal mission, supporting ground validation sites shall deliver spectra and runlogs collected on days of coincident overpasses or enabled Target mode observations at those sites to a Caltech TCCON repository.

L3-Val-50: During the OCO-2 nominal mission, primary ground validation sites shall deliver all raw data to a Caltech TCCON repository.

L3-Val-51: The Caltech TCCON repository shall retain data ingested from primary and supporting ground validation sites for greater than or equal to 6 months after the end of the nominal OCO-2 mission.

2. Ground-based FTS X_{CO2}

A network of ground-based, solar-viewing FTS systems, distributed at various sites throughout the world [**L3-Val-23, L3-Val-24**], has been established in part to facilitate validation of the OCO and OCO-2 instruments. This network, described in more detail below, is known as the Total Carbon Column Observing Network (TCCON) and is coordinated by Paul Wennberg and Debra Wunch at Caltech in Pasadena, CA (https://tccon-wiki.caltech.edu/); David Griffith at the University of Wollongong in Wollongong, Australia and Justus Notholt at the University of Bremen in Bremen, Germany.

Wunch et al, [2010] discusses how TCCON FTS X_{CO2} are calibrated to the WMO atmospheric CO_2 standard [**L3-Val-26**] via over-flights of TCCON sites by aircraft carrying instruments that acquire in situ CO_2 measurements tied to the WMO standard. Regressions of FTS X_{CO2} vs. integrated aircraft in situ CO_2 columns (aircraft X_{CO2}) allow straightforward calibration of the FTS measurement, providing a "standard" that ties measurements of column CO_2 to the WMO standards for in situ point measurements of CO_2 that have long been used by the global carbon science community.

Data from the ground based FTS instruments provide the transfer standard between the data from OCO-2 and the aircraft measurements. A direct comparison between the OCO-2 flight instrument and an upward-looking FTS will be performed during instrument ("Thermal vacuum") testing, when simultaneous data is collected along the same atmospheric optical path with the instrument and a co-located solar-pointed FTS [**L3-Val-32, L3-Val-33**]. This testing is planned for late 2011 and early 2012 at JPL and the upward looking FTS (TCCON) instrument has been periodically taking data at the JPL site since June 2011.

The on-orbit Validation strategy includes an Observatory point-and-stare Target mode, in which the Observatory acquires thousands of observations over a fixed surface site, as it flies over the site. Target mode data acquired over FTS validation sites and the resulting comparisons between the ground-based and space-based data will provide powerful tests of the OCO-2 measurement/retrieval system and provide a mechanism to further establish traceability between WMO-calibrated FTS X_{CO2} on OCO-2 X_{CO2} [**L3-Val-26**]. The Target mode data will provide data that allows a thorough regression analysis and a rigorous quantitative assessment of the errors in the OCO-2 regional X_{CO2} retrieval and provide an understanding of the dependence of any bias on parameters such as solar zenith angle, viewing geometry and/or meteorological conditions [**L3-Val-34**]. Performing the regression and error analysis allows for the identification of potential sources of bias (e.g., due to ancillary data), and subsequent calibration of the space-based retrieval.

TCCON data has been used to validate space-based CO_2 measurements made by several instruments [Reuter et al., 2010, Wunch et al., 2011b, Morino et al., 2011, Butz et al., 2011]. This includes a validation analysis of the data from the GOSAT satellite retrieved using the JPL L2 software designed for the original OCO instrument. This effort lead to a dataset called the Atmospheric CO_2 Observations from Space (ACOS). Validation of the ACOS X_{CO2} data is described in Wunch et al. [2011b] and provides the "road map" for validation of OCO-2 data using TCCON data. This will be discussed in more detail in Section 3.

2.1 The FTS Validation Network

2.1.1 Description

The pre-launch validation activities for the original OCO instrument focused on establishing a network of ground-based, solar-viewing FTS systems distributed at various sites throughout the world. The TCCON network currently (as of August 2011) takes data at 17 different sites, including the new JPL site. The TCCON network is described in detail by Wunch et al., [2011a]. Each TCCON site uses Bruker 125HR instruments, with many of the spectrometers at the primary sites purchased by the OCO/OCO-2 projects. The OCO-2 project has also supported the upgrade of several existing FTS sites to enable data collection in the near infrared CO_2 and O_2 bands used by OCO-2 [**L3-Val-25**]. The site selection process considered factors such as environmental conditions at each site, the ancillary observations of H_2O, temperature, aerosol properties, and carbon cycle related parameters available at each site, and the ability to work with a local liaison who is an established scientist in atmospheric remote sensing.

The FTS validation sites are categorized as either “Primary” or “Supporting” sites depending on a range of factors including data access and availability and importance to the overall Validation effort. Table 2-1 summarizes the characteristics of each category. The primary sites define the minimum set required to characterize biases in the exploratory X_{CO2} data product within 90 days after the end of the IOC (In-Orbit Check-out) [**L3-Val-37**]. Data from the primary and supporting sites will be used to validate the full X_{CO2} data product that will be delivered at the end of OCO-2 science operations.

Table 2-1. TCCON FTS Site Classification

Site Classification	Characteristics
Primary Sites	• Dedicated to X_{CO2} measurements • Supported by OCO-2, NASA • OCO-2 project responsible for calibration to WMO standard, including provision of aircraft over-flights • CO_2 and O_2 measured in same spectral regions as OCO-2 • Frequent target mode observations
Supporting Sites	• Dedicated to X_{CO2} measurements • Not directly supported by OCO-2 or NASA • Calibrated to WMO standard by aircraft over-flights • CO_2 measured in same spectral regions as OCO • Less frequent Target mode observations

2.1.2 Driving Requirements and Goals – FTS Validation Network

The following requirements apply specifically to the TCCON network, the data it produces and how those data are used for OCO-2 validation.

L1-REQ-9: Compare space-based and ground-based X_{CO2} retrievals from soundings collected during over-flights of ≥ 3 primary ground validation sites at least once each season to identify and correct global-scale systematic biases in the space-based X_{CO2} product and to demonstrate a precision of $\leq 0.3\%$ for collections of ≥ 100 cloud-free soundings.

L3-Val-23: The OCO-2 space-based retrievals shall be validated using observations from at least 7 FTS validation sites, selected to span a range of latitudes and longitudes.

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L3-Val-26: The NOAA ESRL CO_2 standard shall be used for calibration of the ground-based FTS systems.

L3-Val-27: The ground-based FTS instruments used for OCO-2 validation shall be operated with a HCl cell installed during data acquisition.

L3-Val-28: Each primary FTS validation site shall be calibrated by aircraft in situ CO_2 observations from the boundary layer to the middle troposphere (≥10 km altitude) at least once prior to the end of the OCO-2 science mission.

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L3-Val-32: During pre-launch testing of the flight instrument, simultaneous data will be collected along the same atmospheric optical path by a co-located, solar-looking FTS.

L3-Val-33: During pre-launch testing of the flight instrument, the spectra simultaneously acquired from the collocated flight instrument and ground-based FTS shall be analyzed using the same retrieval algorithm to define the level of agreement between measurements of X_{CO2} from the two systems.

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L3-Val-35: The validation team shall compare X_{CO2} retrievals from OCO-2 Target Observations with coincident X_{CO2} retrievals from the targeted FTS validation site.

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L3-Val-37: The validation team shall quantify biases in the exploratory X_{CO2} data product within 90 days of the end of IOC.

L3-Val-38: The validation team shall request ≥9 target opportunities for each primary validation site during the first year of science operations.

L3-Val-39: To enable a planned Target Observation, the validation team shall submit a CAR to the MOC at least two hours prior to the uplink pass preceding the Target Observation.

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L3-Val-50: During the OCO-2 nominal mission, primary ground validation sites shall deliver all raw data to a Caltech TCCON repository.

L3-Val-51: The Caltech TCCON repository shall retain data ingested from primary and supporting ground validation sites for greater than or equal to 6 months after the end of the nominal OCO-2 mission.

2.1.3 Plan

OCO-2 requires the continued operation of a ground-based X_{CO2} remote sensing network calibrated to the WMO CO_2 standard to meet its baseline mission [**L1-REQ-7**], Level 1 Science Measurement Validation Requirements [**L1-REQ-9**], and lower level Science/Validation requirements [**L3-Val-23, 30, 31**]. Funding for the Primary sites comes from the OCO-2 Project, NASA, or is covered via working agreements within the TCCON network; all other sites are funded outside the OCO-2 Project.

The OCO-2 Validation team which includes the TCCON team at Caltech, will interface with TCCON network site principal investigators to insure the following tasks are completed throughout the lifetime of the project:

- Maintain TCCON standards, measurement protocols and data quality
- Constant, rigorous calibration and bias removal for TCCON measurements
- Coordinate Target Observations with the OCO-2 Project and TCCON site PIs
- Provide ground-based X_{CO2} data calibrated to the WMO standard

The OCO-2 project working with Caltech is responsible for maintaining the FTS instruments located at JPL (during instrument testing), Park Falls, WI, Lamont, OK and Darwin, Australia. The Atmospheric Radiation Monitoring (ARM) program provides infrastructure and technical support for the OCO-2 FTSs at Lamont and Darwin. The agreement with the ARM project for support of FTS containers at Darwin and Lamont has been extended through 2016. The FTS at Lauder, New Zealand is committed to supporting OCO-2 as part of the TCCON network. These sites (Darwin, Lauder, Park Falls and Lamont) constitute the Primary FTS validation sites [**L3-Val-24**] and are the minimum set required to characterize the exploratory X_{CO2} data product that will be released within 90 days after the end of the IOC [**L3-Val-37**].

Individual TCCON site principal investigators will be responsible for all operations, maintenance, data acquisition, and calibration at their sites. They will also be responsible for providing status updates on instrument readiness and coordinating OCO-2 Target observations with the OCO-2 validation team.

2.1.4 TCCON Network Status

The FTS sites supporting OCO-2 validation are part of the Total Carbon Column Observing Network (TCCON). TCCON presently consists of 17 stations worldwide (Figure 2-1). Details of the site selection criteria, site capabilities, ancillary data measurements, etc. are given in the Appendix. The most up-to-date TCCON information may be found at https://tccon-wiki.caltech.edu/.

Figure 2-1 shows a map of the location of TCCON FTS validation sites active as of November 2011. The network was initiated with the installation of an automated observatory at the WLEF tall tower site in Park Falls, Wisconsin in May 2004. The network has expanded rapidly, due to support from NASA as well as international agencies. Details of station locations and investigators can also be found at https://tccon-wiki.caltech.edu/ and in Table 2-2. Several sites are expected to be operating by the time OCO-2 is launched, these include Ascension Island, Reunion Island, Four Corners, NM and Pasadena, CA (on the Caltech campus).

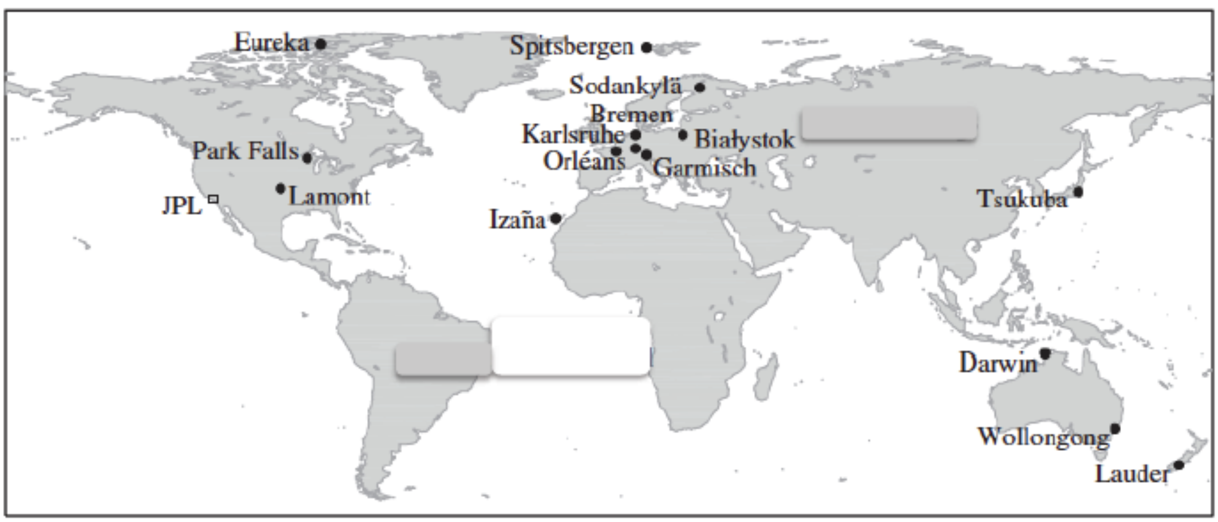

Figure 2-1. A map of the FTS validation sites planned for OCO-2 use, active as of November 2011. The sites span a range of latitudes and hemispheres and sample both oceans and continents. The Primary sites (Park Falls, Lamont, Darwin, and Lauder) are the minimum set required to characterize the Exploratory X_{CO2} data product.

Table 2-2 List of active TCCON sites as of August 2011.

Site	Established	Latitude	Longitude	Altitude (km)
Bialystok, Poland	March 2009	53.23N	23.025E	0.18
Bremen, Germany	July 2004	53.10N	8.85E	0.04
Darwin, Australia	August 2005	12.424S	130.892E	0.03
Eureka, Canada	August 2006	80.05N	86.42W	0.61
Garmisch, Germany	July 2007	47.476N	11.063E	0.74
Izana, Tenerife	May 2007	28.3N	16.5W	2.37
Karlruhe, Germany	September 2009	49.1N	8.438E	0.11
Lamont, Oklahoma	July 2008	36.604N	97.486W	0.32
Lauder, New Zealand**	June 2004 February 2010	45.038S	168.684E	0.37
Ny Alesund, Spitsbergen	April 2002	78.9N	11.9E	0.02
Orleans, France	August 2009	47.97N	2.113E	0.13
Park Falls, Wisconsin	May 2004	45.945N	90.273W	0.44
Pasadena, California	June 2011	34.2N	118.18W	0.39
Sodankyla, Finland	January 2009	67.368N	26.633E	0.18
Tsukuba, Japan	December 2008	36.0513N	140.1215E	0.03
Wollongong, Australia	May 2008	34.406S	150.879E	0.03

* Note that the Ascension Island FTS was on campaign in Wollongong, Australia.

** Lauder has two instruments, the 120 HR instrument has been operational since June 2004, the 125 HR has been operational since February 2010.

2.1.5 Primary Sites

The primary sites are stations dedicated to the measurement of X_{CO2} that are either supported directly by OCO-2 or working through the TCCON charter as managed by the TCCON team. The OCO-2 project is responsible for calibrating the FTS measurement of X_{CO2} to the WMO standard [**L3-Val-28**] by analyzing in situ CO_2 profiles over each primary site. The instruments at the primary sites must have the capability to obtain measurements in the three spectral regions used by the OCO-2 flight instrument [**L3-Val-25**] and all four primary sites currently have the detectors in place to make those measurements

OCO-2 validation requires at least one aircraft over-flight of each primary site prior to the completion of the OCO-2 mission to provide calibration to the WMO standard [**L3-Val-28**]. In fact, calibration flights have already been conducted over all Primary sites (Lamont, Darwin, Lauder and Park Falls), [Wunch et al., 2010] and the network is fully calibrated to the aircraft standard, [Wunch et al., 2011a]. Use of the AirCore balloon system, which can provide vertical profiles of CO_2, at least for the Lamont and Park Falls sites remains a possibility for future calibration of the TCCON data to the WMO standard.

Target observations will be conducted over the primary sites as often as possible during the mission, with at least 9 target mode observation requests, per site, during the first nine months of science operations [**L3-Val-38**]. A key component of the validation analysis is capturing data to examine the seasonal variation in X_{CO2} and the nine Target observations per year over each primary site provide sufficient data to achieve this goal. Orbit simulations provided to the OCO-2 Validation team by the OCO-2 Mission Operations team suggest that the primary sites can be targeted at least 4 times (elevation greater than 60 degrees) every 16 days, allowing ample opportunities for meeting the target observation requirements.

2.1.6 Supporting Sites

The supporting sites for OCO-2 validation are stations that are dedicated to the measurement of X_{CO2} but are not supported by OCO-2 or NASA funding. Supporting sites are expected to deliver data of similar quality to the primary sites.

Target observations will be conducted over these sites less frequently than over the primary sites, with target decisions made based on an assessment of data quality from each station and the need to obtain target measurements at stations that have different characteristics (i.e., surface reflectivity, aerosol environment, etc) than the primary sites.

The OCO-2 program *will not* be responsible for acquiring aircraft over-flights for supporting sites, but will encourage such over-flights based on existing collaborations.

2.1.7 Future sites

Several new sites could potentially join the TCCON network in the future. These sites will be categorized as supporting sites.

2.1.8 Implementation

The TCCON network of ground based instruments has grown significantly since the launch of OCO. The primary sites are operational and ready to meet the OCO-2 validation requirements. The Caltech OCO-2 validation team shall provide a TCCON data repository that will store data from the different TCCON sites. The primary sites will archive all raw data, runlogs, a priori information, averaging kernels, surface pressure measurements and X_{CO2} data at Caltech. Supporting sites will deliver the a priori information, averaging kernels, surface pressure measurements and X_{CO2} data to Caltech. Supporting sites will also deliver runlogs and spectra on days during which their sites have been observed using OCO-2 target mode. Since 2009, the Caltech OCO-2 Validation/TCCON team has been acting as a provider of ground based FTS data through their TCCON database, and is in the best position to obtain, handle and archive the various levels of data from the different sites.

2.2 FTS X_{CO2} Calibration with Aircraft In Situ CO_2 Profiles

2.2.1 Description

FTS X_{CO2} will be calibrated to the WMO atmospheric CO_2 standard via over-flights of the OCO-2 FTS validation sites [**L3-Val-26, L3-Val-28**] by aircraft carrying instruments that acquire in situ CO_2 measurements from the boundary layer to the middle troposphere, (i.e., to at least 10 to 15 km altitude) [**L3-Val-28**] tied to the WMO standard [**L3-Val-29**]. Regular FTS calibration over-flights began in the summer of 2004 [**L3-Val-28**] and will continue throughout the OCO-2 mission life. Regressions of FTS X_{CO2} vs integrated aircraft in situ CO_2 columns (aircraft X_{CO2}) allow straightforward calibration of the FTS measurement, as demonstrated using GOSAT/ACOS X_{CO2} retrievals [Wunch et al., 2010]. The calibration of the ground based data using aircraft measurements is the key to linking measurements of *column* CO_2 to the WMO standards for in situ *point* measurements of CO_2 that have long been used by the global carbon science community [**L3-Val-26**].

2.2.2 Driving Requirements and Goals

L3-Val-26: The NOAA ESRL CO_2 standard shall be used for calibration of the ground-based FTS systems.

L3-Val-28: Each primary FTS validation site shall be calibrated by aircraft in situ CO_2 observations from the boundary layer to the middle troposphere (≥10 km altitude) at least once prior to the end of the OCO-2 science mission.

L3-Val-29: The aircraft in situ observations of CO_2 shall be traceable to the NOAA ESRL standard.

2.2.3 Status

The calibration of the TCCON network is discussed in detail in Wunch et al. [2010]. Calibration flights over the Primary FTS validation sites will be planned at least once every 24 months during OCO-2 science operations to avoid the uncertainties associated with extrapolating the FTS calibration more than 4-5 ppm. The list of calibration flights as of the publication of Wunch et al. [2010] is provided in Table 2-3 of the paper and reproduced below in Table 2-3. Some funding for the calibration flights over the Primary FTS validation sites will come from the OCO-2 Project or NASA. Calibration flights over all other sites are funded outside the OCO-2 Project.

Table 2-3 List of aircraft flights over TCCON stations including all four primary sites [Wunch et al., 2010].

Site	Aircraft Campaign	Dates	References
Park Falls	INTEX-NA COBRA START-08	Jul/Aug 2004 May 2008	Washenfelder et al., JGR 2006
Darwin	TWP-ICE HIPPO-5	Feb 2006 August 2011	Deutscher et al., AMT, 2010

Site	Aircraft Campaign	Dates	References
Lamont	HIPPO-1,2,3 Lear	Jan 2009 Aug 2009	Wunch et al., AMT, 2010
Lauder	HIPPO-1,2,3	Jan 2009	Wunch et al., AMT, 2010
Tsukuba	King Air	Jan 2009	Wunch et al., AMT, 2010

A typical aircraft profile of CO_2 obtained over a validation site, which yields an estimate for X_{CO2} of 373.6 ± 0.52 ppm, is shown in Figure 2-2. In general, the largest contributor to the uncertainty in this estimate of column CO_2 is attributed to the abundance of CO_2 above the aircraft data (for the flight in Figure 2-2, this means pressures less than 200 mbar). The aircraft profiles are combined with a priori values from the TCCON retrieval algorithm (GFIT) to define values of X_{CO2} that to the top of the atmosphere [Wunch et al., 2010].

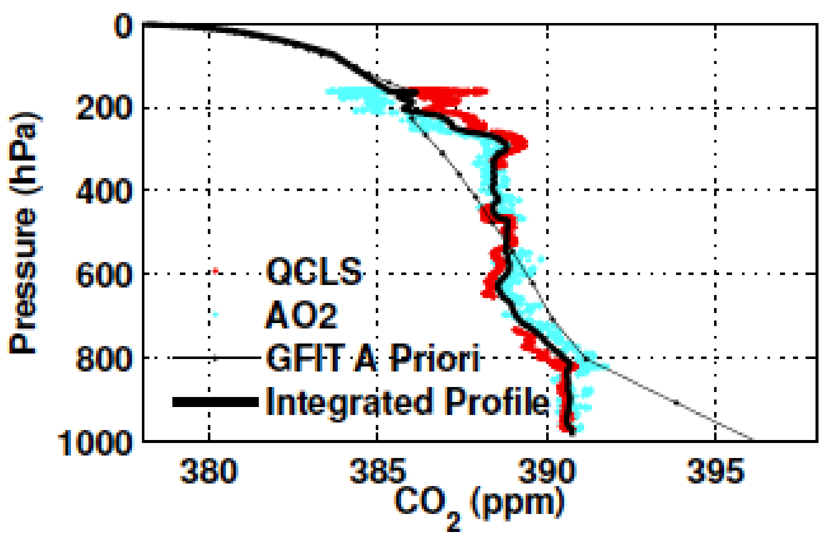

Figure 2-2 Taken from **Figure 2** in Wunch et al. [2010]. Shown is the combined aircraft CO_2 profile over Lamont from a 30 January 2009 HIPPO overpass. The colored dots show the aircraft data. The thin black line shows the GFIT a priori profile for 30 January 2009 over Lamont. The thick black line is the profile that is integrated.

Several aircraft over-flights of the OCO-2 FTS sites have demonstrated the precision and stability of the FTS method. Washenfelder et al. [2006] documented efforts to calibrate the TCCON X_{CO2} measurements to the WMO CO_2 mole fraction standard prior to the launch of OCO [**L3-Val-28**]. Wunch et al. [2010] completed the calibration analysis and the plots of FTS X_{CO2} versus aircraft X_{CO2} demonstrate that measurements of column CO_2 from the OCO-2 FTS instruments define a compact regression. The scatter about the regression line is < 0.15 ppm (0.05%), significantly better than the 1 ppm (0.3%) requirements for the space-based OCO-2

X_{CO2} data (Figure 2-3). Excellent precision is achieved and the numbers are provided in **Table 5** of Wunch et al. [2010].

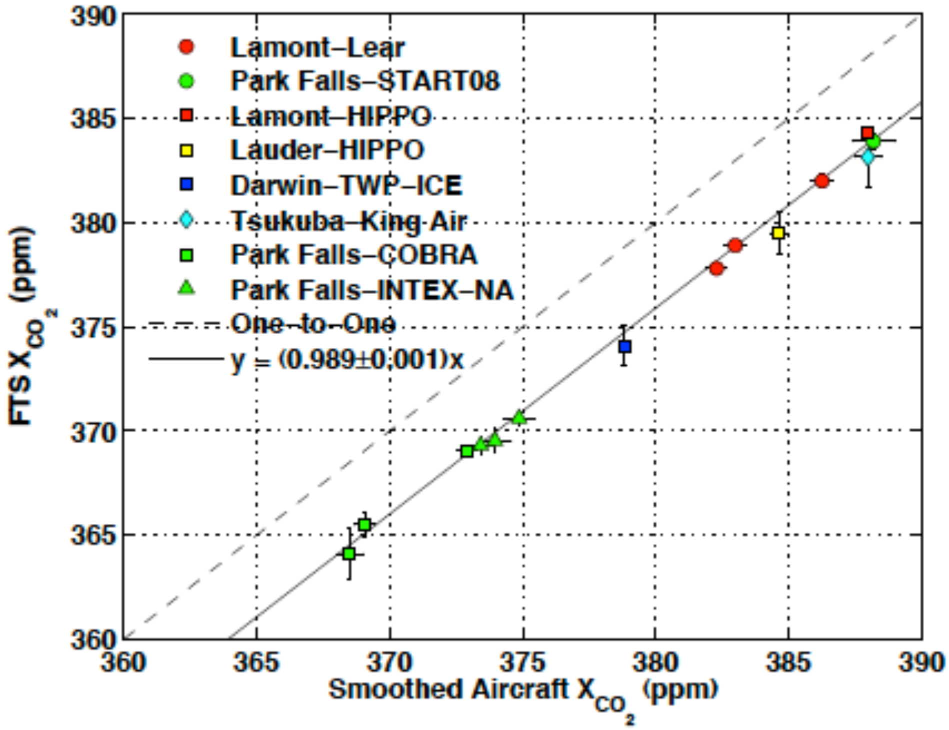

Figure 2-3. The calibration curve for CO_2 from Wunch et al. [2010] showing the excellent correlation between aircraft and ground based measurements. There is a slight offset to the data.

The small, residual bias between TCCON X_{CO2} and aircraft X_{CO2} is the subject of concerted, on-going investigation by the OCO-2 team. The Figure 2-3 scatter plot of X_{CO2} from the Park Falls TCCON site versus X_{CO2} from the in situ measurements shows the data are offset from the one to one line by about 1%. TCCON measurements of X_{CO2} will be corrected for this small bias using aircraft calibration flight data (empirical *correction*). An example is shown in Figure 2-4, where the measurements of X_{CO2} from the Park Falls FTS have been "calibrated" to result in no residual bias with respect to the aircraft data. The goal is to pursue a "spectroscopic" solution to the slight residual (*physics-based correction*) while, at the same time, having an "empirical" solution available for use in the validation of the space-based retrieval.

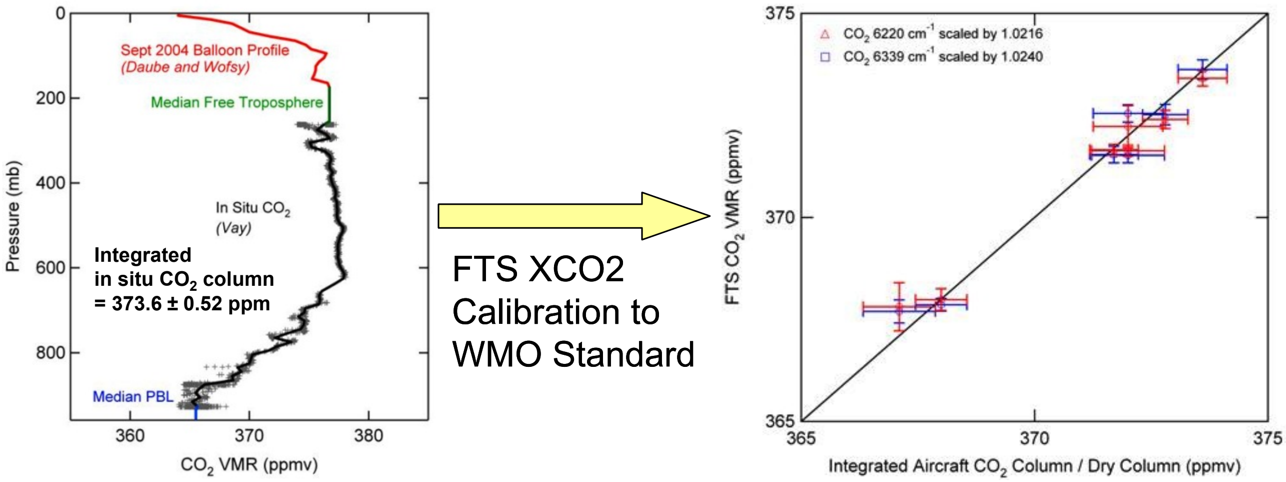

Figure 2-4. Integrated in situ CO_2 aircraft profiles measured over Park Falls, WI in summer 2004 were used to calibrate FTS X_{CO2} retrievals to the WMO standard [**L3-Val-29**]. The scatter of the points about the 1:1 correlation line is < 0.2 ppm (0.05%), significantly better than the requirements for the space-based X_{CO2} product.

Vertical information from the balloon-borne measurements, such as the AirCore instrument, could also provide a cost effective means for supplementing the aircraft flights at Lamont and Park Falls [Karion et al., 2010]. A planned test flight of the AirCore system is planned for early 2012, if successful; the AirCore measurements could be incorporated into the plan for maintaining the calibration of some TCCON sites. Vertical profiles of CO_2 from the AirCore balloon system remain a possible source of data for future calibration of the TCCON measurements to the WMO standard (at least for the Lamont and Park Falls sites). If, as expected, the AirCore data can provide vertical profile information, similar to the aircraft, it will provide a means of mitigating risk to the science validation effort that may occur as a result of potential OCO-2 launch delays. It could also provide a cost effective means for supplementing the aircraft data used for calibration of the TCCON network.

2.3 Heliostat/FTS Observations

2.3.1 Description

The ground based FTS systems have 15-35 times higher spectral resolution than the space-based spectrometers (~0.02 cm^{-1} resolution for the ground-based FTS, compared to values in the range 0.2 to 0.7 cm^{-1} for the space-based spectrometers). As a result, the averaging kernels (a metric of the degree and vertical location of the sensitivity in the observations) of the two measurements of X_{CO2} differ, with the averaging kernel for the ground-based FTS being near unity at all altitudes (due to the high spectral resolution of the measured radiances) and the averaging kernel of the OCO-2 measurement of X_{CO2} peaking near the surface. The averaging kernels of the ground-based FTS systems and the OCO-2 flight instrument are calculated using a radiative transfer model, and so factor into all comparisons of X_{CO2} measurements from these two types of spectrometers.

The accuracy of the calculated averaging kernels is verified by comparison of side-by-side measurements of X_{CO2} from one of the FTS systems and the actual space-based spectrometer, obtained on the ground at JPL prior to launch [**L3-Val-32, L3-Val-33**]. This side-by-side comparison of column CO_2 and column O_2 measurements from the two types of spectrometers is vital for assessing a host of other spectroscopic issues related to the flight instrument.

The direct comparison between the flight instrument and upward-looking FTS is accomplished during instrument testing, when simultaneous data is collected along the same atmospheric optical path with the instrument and the co-located solar-looking FTS. A new Bruker 125 HR and container were assembled at JPL in early 2011 and have been taking data periodically since June 2011. This instrument will provide the upward looking capability for the instrument testing.

2.3.2 Driving Requirements and Goals

L3-Val-32: During pre-launch testing of the flight instrument, simultaneous data will be collected along the same atmospheric optical path by a co-located, solar-looking FTS.

L3-Val-33: During pre-launch testing of the flight instrument, the spectra simultaneously acquired from the collocated flight instrument and ground-based FTS shall be analyzed using the same retrieval algorithm to define the level of agreement between measurements of X_{CO2} from the two systems.

2.3.3 Plan

The required simultaneous data collection from the OCO-2 flight instrument and the co-located solar-pointed FTS are scheduled to begin in October 2011. All resources required for the heliostat observations will be committed by the OCO-2 Project during Phase C/D. The science validation team will work with the OCO-2 calibration team to support the thermal vacuum tests.

3. Establishing WMO Traceability for X_{CO2} on Regional Scales

3.1 Description

Target mode observations of TCCON sites, plus coincident nadir measurements will provide the initial set of data that allow for the validation of the OCO-2 data and the connection of the space based X_{CO2} data to the WMO standard [**L1-REQ-9, L3-Val-25, L3-Val-29, L3-Val-30**]. Validation in the early stages of the OCO-2 mission will be performed doing regression analysis similar to that described in Wunch et al. [2011b]. In that paper, the TCCON data was used to evaluate systematic errors in the ACOS retrievals of GOSAT radiances. The approach uses the general uniformity of column CO_2 south of 25°S to identify large biases in the ACOS data. In the Northern hemisphere, the amount of validation data is increased by making use of the correlation between free tropospheric temperature and X_{CO2} and thereby defining better coincidence criterion. A regression analysis performed after accounting for the systematic errors illustrates different parameters within the retrievals that lead to an improvement in the data. The use of the correlation between atmospheric temperature and X_{CO2} will be useful for OCO-2 analysis, though the use of Target Mode observations will provide a much larger set of coincident data than what was used in the ACOS analysis. The methods described in Wunch et al. [2011b] will be the basis of the validation effort for OCO-2 data.

3.2 Driving Requirements

L1-REQ-9: Compare space-based and ground-based X_{CO2} retrievals from soundings collected during overflights of ≥ 3 primary ground validation sites at least once each season to identify and correct global-scale systematic biases in the space-based X_{CO2} product and to demonstrate a precision of ≤ 0.3% for collections of ≥100 cloud-free soundings.

L3-Val-30: At primary validation sites, the ground-based FTS instruments shall have a clear-sky rms calibrated X_{CO2} accuracy of <=0.3% for soundings taken within +/- 30 minutes of a targeted overflight.

L3-Val-31: The validation team shall demonstrate validation of the OCO-2 space-based surface pressure retrievals over oceans and topographically flat regions to an accuracy ≤ 1 mbar.

L3-Val-34: The validation team shall quantify the bias in space-based X_{CO2} retrievals as a function of geophysical and observation variables, including humidity, temperature, solar zenith angle, and aerosol optical depth.

L3-Val-35: The validation team shall compare X_{CO2} retrievals from OCO-2 Target Observations with coincident X_{CO2} retrievals from the targeted FTS validation site.

L3-Val-36: The validation team shall demonstrate comparison of space-based X_{CO2} retrievals with coincident X_{CO2} retrievals from FTS validation sites.

L3-Val-37: The validation team shall quantify biases in the exploratory X_{CO2} data product within 90 days of the end of IOC.

L3-Val-38: The validation team shall request ≥9 target opportunities for each primary validation site during the first year of science operations.

L3-Val-39: To enable a planned Target Observation, the validation team shall submit a CAR to the MOC at least two hours prior to the uplink pass preceding the Target Observation.

3.3 Plan

OCO-2 requires Target observations of the ground-based FTS X_{CO2} remote sensing network to link OCO-2 space-based X_{CO2} to the WMO-calibrated FTS network and hence the WMO in situ CO_2 standard to meet its baseline mission requirements.

The JPL Validation Team in conjunction with the Caltech members of the Validation/TCCON team and the OCO-2 Mission Operations team will coordinate the planning of Target mode observations. The JPL and Caltech members of the Validation team will work together to analyze data taken in Target mode and provide bias estimates for the coincident data. Coincidence criteria will be determined by studying coincidences in the ACOS retrievals of the GOSAT data.

3.4 Implementation

3.4.1 Overview of Methodology

To meet the Level 1 mission requirement that all random errors and systematic biases in OCO-2 X_{CO2} are reduced to less than 0.3% (1 ppm) on regional scales [**L1-REQ-9**] the validation team will rigorously characterize all sources of geophysical bias through comparisons with the ground based data and regression analysis to reduce variance in X_{CO2} anomalies seen in Southern hemisphere data. The reason for using the Southern hemisphere to evaluate a bias in the satellite data is that model and observations of total CO_2 column show low seasonal and geographic variability compared to the Northern hemisphere [Wunch et al., 2011b, Wofsy et al., 2011]. This allows for an evaluation of potential bias in the satellite data while minimizing the effects of atmospheric variability.

3.4.2 Target Mode Observations

The OCO-2 spacecraft is designed to support three pointing modes: nadir, glint, and target. The main driver behind the design of Target mode was the opportunity to maximize the number of coincident observations of X_{CO2} over the FTS sites. Coincident observations are key to providing traceability between the WMO-standard-calibrated FTS X_{CO2} measurement and the OCO-2 space-based Regional X_{CO2} retrieval. During Target mode observations, the spacecraft will point the instrument boresight at a surface target as it flies overhead, acquiring observations at surface zenith angles ranging from 0° to 75°. Target passes typically last up to 9 minutes, providing more than 6000 soundings in the vicinity of the target. This large number of soundings reduces the impact of random errors and provides opportunities to identify spatial variability in the X_{CO2} field near the target. Most importantly, Target mode measures X_{CO2} at a variety of viewing angles over a fixed ground location (e.g., constant X_{CO2} during the overpass). Target observations over a range of latitudes will provide opportunities to identify and correct for biases associated with observing geometry as well as a range of geophysical parameters.

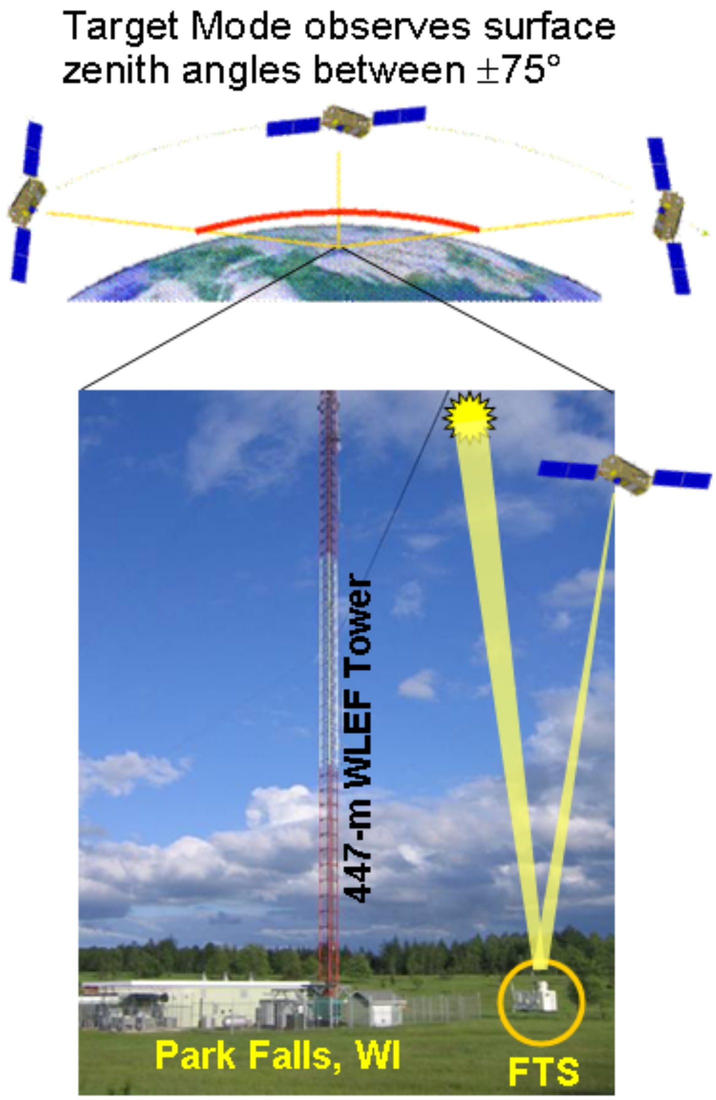

Figure 3-1. Illustration showing Target mode geometry

Orbit track simulations indicate that there will generally be greater than four (in many cases more) opportunities every 16 days to obtain Target mode observations over each site. The time involved in executing the switch to Target mode, and then back to Nadir or Glint, will result in few non-Target observations being obtained for the particular orbits in which Target mode is enabled. The decision to enable Target mode, then, will be based on the weather forecast at each site, the FTS operational status, the overall progress of the validation effort, etc to maximize the number of coincident observations at various viewing angles. There are 19 locations that can be targeted by OCO-2 that are implemented in the Relative Time Sequences (RTS) and Mission Planning System (MPS). If absolutely necessary, these RTS locations can be swapped out, but a stable, final set of the locations will be determined prior to launch. The Mission Operations team will provide a Target Opportunity File that will provide the possible target locations for the next day. Based on weather forecasts, the amount of data already obtained for a ground based site, the Validation team will submit a request for a particular target observation. The Mission Operation's plan allows for science team members to submit requests for Target mode enable up to (but no later than) two hours prior to the uplink pass preceding the desired Target observation.

Target mode observations are required from nine successful sets of target observations over each of the four primary validation sites during the first year of operations – with a goal of obtaining at least one Target mode set of data over every primary OCO-2 FTS validation site (i.e., Lamont, Park Falls, Darwin, and Lauder) each month during the first year. Simulations of the OCO-2 orbit tracks suggest that overpasses for the primary validation sites occur frequently enough that there should be no problem in meeting this requirement. Additional Target mode opportunities are desirable but not required. Target observations over supporting validation sites will be performed as warranted based on an evaluation of the TCCON-reported accuracy of the retrievals of X_{CO2} at each site, and the need for targets at more geographic locations determined by the Validation team (e.g., to add robustness to the validation effort or provide a diagnostic assessment of the slit misalignment corrective algorithm).

During the first month of science operations, the Validation team will request at least one Target observation over each of the four Primary FTS validation sites (weather permitting). The Validation team will provide updates consisting of plots that quantify biases from the X_{CO2} retrievals from the OCO-2 Full Physics algorithm. These updates will be distributed to the OCO-2 science team via email and discussed during a weekly telecon expected to take place during at least the first three months of operation. Efforts during the first month will focus on quantifying and removing biases related to viewing angle.

3.4.3 Coincident Observations near FTS Validation Sites

Inherent to the OCO-2 validation process is the examination of data from the space-based instrument that are coincident, in space and time, with observations from the ground based FTS network [**L1-REQ-9, L3-Val-30**]. Coincident criteria for ACOS GOSAT retrievals are described in Wunch et al. [2011b] and set differently for different Northern hemisphere sites. The temperature at 700 hPa is used to increase the number of coincident measurements. OCO-2 will provide a much larger set of coincident data which might allow for tightening the coincidence criteria, though the values set in Wunch et al. [2011b] could be used as a starting point.

4. OCO-2 L2 Retrieval Algorithm Testing and Preliminary Validation

4.1 Description

Since the launch failure of the OCO instrument, both the retrieval algorithm and validation analyses have been refined as a part of the ACOS task. In addition, a system of testing the algorithm has been developed that includes validation analysis. This has allowed for an interaction between the algorithm and validation teams that have been beneficial to both efforts. The analysis of retrieved results during software testing has allowed the validation team to identify specific quantities of interest, critical to properly evaluating and validating the column CO_2 data. The testing of the retrieval results has provided feedback to the algorithm team for areas in the software that need to be improved or upgraded. The ACOS task has allowed both teams to develop a system where they work together to provide a preliminary validation of the retrieval results prior to finalizing a build. The results from the ACOS task (described below) will be applied during the mission lifetime and will be a critical part of the validation plan for OCO-2 data.

The ACOS task uses the OCO-2 Level 2 retrieval algorithm and data from the Greenhouse gases Observing Satellite (http://www.jaxa.jp/projects/sat/gosat/index_e.htm, GOSAT) developed jointly by the Japan Aerospace Exploration Agency (JAXA) and Japan's Ministry of the Environment (MoE). GOSAT carries two instruments. The TANSO-FTS is a Fourier transform spectrometer that records spectra in narrow SWIR (Shortwave Infrared) bands to detect O_2 (12900–13200 cm^{-1}), CO_2 (4800–5200 cm^{-1}) and CH_4 and CO_2 (5800–6400 cm^{-1}) as well as a wide TIR (Thermal Infrared) band (700–1800 cm^{-1}) with 0.2 cm^{-1} resolution. The TANSO-CAI is a UV-VIS-NIR (Ultra Violet – Visible - Near Infrared) imager designed to identify cloud and aerosol interference in the TANSO-FTS radiances. The instruments have a 10.3 km FOV (Field of View) at nadir and a mirror that can scan ±35° across the ground track to create a 90 to 800 km wide mapping of the surface. The orbit has an inclination of 98.05° resulting in a 3-day/44 orbit repeat cycle with 8.2° longitude between adjacent orbits. The GOSAT team will retrieve measurements of total column CO_2, CO, and CH_4. The ACOS project has focused only on retrievals of CO_2.

4.2 Driving Requirements and Goals

Goal: Utilize testing procedures developed during the ACOS task to provide validation type analysis during development of updates to the retrieval algorithm. This will allow the Science team to obtain a better understanding of which aspects of the retrievals could be contributing to biases

Goal: Provide comparisons of X_{CO2} from GOSAT and the OCO-2 retrievals for coincident observations. Preliminary comparisons might use coincident comparisons at the TCCON sites as a "transfer standard".

4.3 Algorithm Testing Plan

A critical component of the work to validate OCO-2 X_{CO2} retrievals involves the relationship between understanding biases in the data and the algorithm that produced the data. The output from the retrieval algorithm provides diagnostic fields that allow the validation team to investigate the effects of atmospheric and surface properties on the retrieved data and bias seen in comparisons to the ground based observations. The validation data set can also be used as part of the process of testing updates and improvements to the retrieval algorithm during the development process.

In addition, an important aspect of providing a data set such as ACOS and OCO-2 is being able to communicate to the data users information on how the data set has evolved. When improvements are made to the retrieval software and new data versions are produced it is vital to provide information to the data users. The validation effort is focused on establishing an understanding of potential biases in the data but should also provide information on the causes of those biases and the effects of efforts to mitigate them.

As part of the ACOS task, the OCO-2 Algorithm and Validation teams worked together to develop a hierarchy of tests that would allow for testing changes to the retrieval software prior to released and implementation of the code. These tests utilized the TCCON data to estimate how changes in the retrieval software would manifest themselves in the observed bias between the GOSAT and TCCON X_{CO2} values. This testing of the retrieval code with a focus on a preliminary "validation" of the results allow for the Algorithm team to understand the effects different code updates have on the results and allow for communication to the users of ACOS data on the evolution of the data set. Similar tests will be performed as part of the OCO-2 algorithm development, update and release cycle. An overview of the tests that were performed during the ACOS task is provided below.

4.3.1 Hierarchy of Algorithm Testing

As part of the ACOS task, the OCO-2 retrieval software evolved in significant ways. The OCO-2 Algorithm and Science teams developed four different levels of tests to better understand the effects of changes on the retrieved results:

1. Regression Testing
2. Enhanced Science Regression Testing
3. Science Acceptance Testing
4. Data Characterization

These tests were run at different points in the development process and were intended to provide different information back to the Science Team. The different levels of testing are described in the next section.

4.3.2 Regression Testing

These tests were part of the standard software development process during ACOS and will be for OCO-2. The goal of these tests is to show how updates to the software affect the retrieved data results. Because there are often many (typically minor) changes during the algorithm development process, this test needs to be run on a small set of data. The validation team put together a set of about 500 GOSAT soundings that corresponded to “clear sky” observations from the TCCON data set. This small set of validation data was used for comparison to data retrievals from intermediate builds of the retrieval and allowed for a quick look at the effects of changes in the software. This process provided a record of the effects on the retrieved X_{CO2} of specific changes to the algorithm (Figure 4-1 and Figure 4-2). The example in Figure 4-1 shows the mean X_{CO2} values for the test set of GOSAT soundings as a function of the changes to the retrieval software. Figure 4-2 shows a similar plot that illustrates the changes in the “bias” between retrieved and true surface pressure for the small test set.

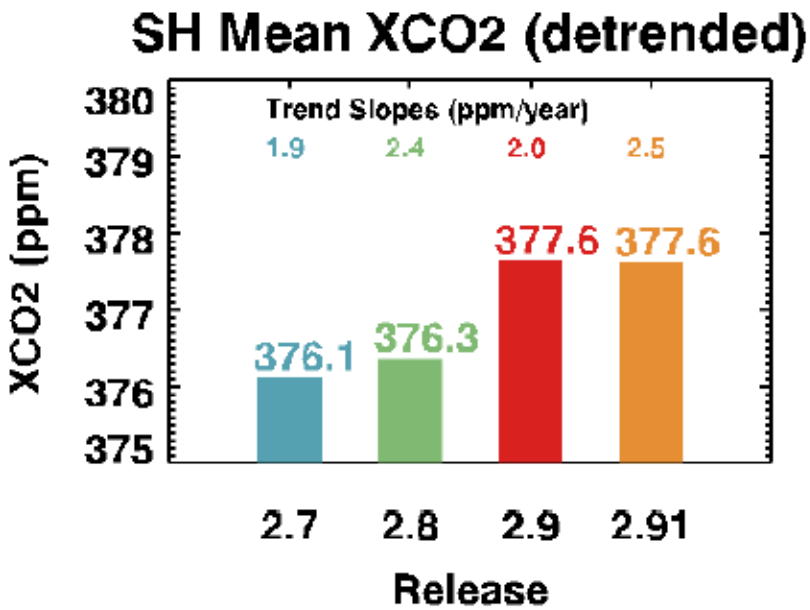

Figure 4-1. Evolution of the mean X_{CO2} value in the Southern Hemisphere for different ACOS releases. The plot allows for an understanding how changes in the software manifest themselves into the data and is meant as an example.

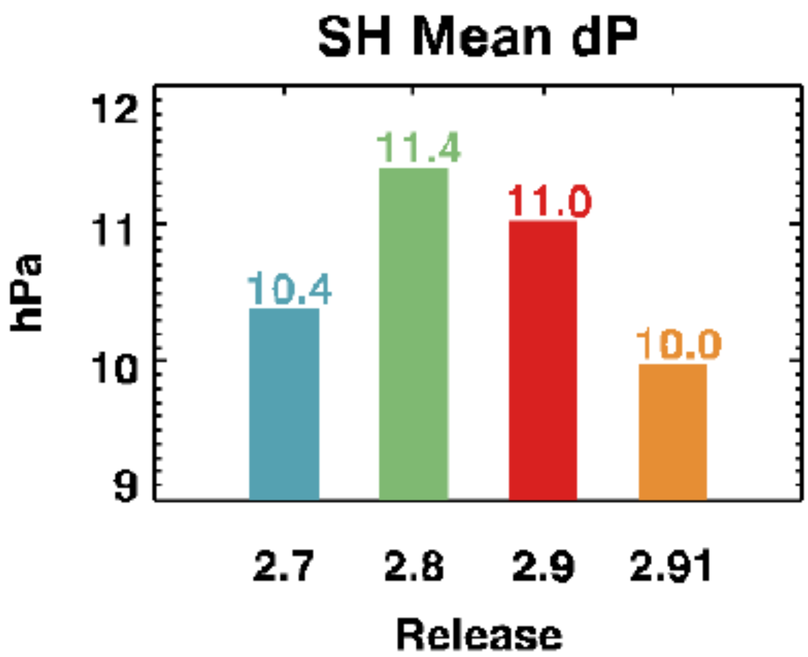

Figure 4-2. An example of the evolution of the mean bias in surface pressure in the Southern Hemisphere for different ACOS releases. These plots will be used in to isolate individual changes in the software during regression testing.

The data set for ACOS regression testing was relatively small, primarily so it could be run quickly, but also due to the relatively small number of TCCON coincidences provided by the GOSAT orbit and footprint size. The set that we use for OCO-2 will be determined in the first 3 months of operation and will include as many TCCON stations as possible, spanning a wide range of latitudes [**L3-Val-23**]. The Target mode data will provide for significantly more data that can be used for regression testing.

4.3.3 Enhanced Science Regression Testing

When an update is incorporated into the retrieval algorithm that is believed to have a significant impact on the retrieved data, it will be run through the "Enhanced" regression testing. This will provide a way of better characterizing the effects of this single change on the retrieved data. The data used will be a larger set of data, but still the results can be turned around quickly to determine if the retrieval results are of the expected quality.

In the case of ACOS testing, the test set included the set of TCCON/GOSAT coincident soundings, a set of southern hemisphere soundings and a set of glint soundings. The total number of soundings was around 10,000. With OCO-2 data and target mode observations, the OCO-2 Algorithm and Validation team will be able to select the test data set to provide improved bias estimation and information, including better estimates of the quality of glint observations.

The product of the enhanced regression testing will provide values for key indicators of retrieval quality in a tabular format to provide a "high level" view of the effects of the software update. These include values such as mean X_{CO2}, mean X_{CO2} bias relative to TCCON, bias in retrieved surface pressure, "chi square" values and other quality indicators. There will be a hierarchy of support plots that support this table of numbers. Again, among the metrics used in making that determination included estimates of the bias relative to the TCCON data (Figure 4-3). The change in the X_{CO2} value compared to the previous data version is also tracked as part of the analysis (Figure 4-4).

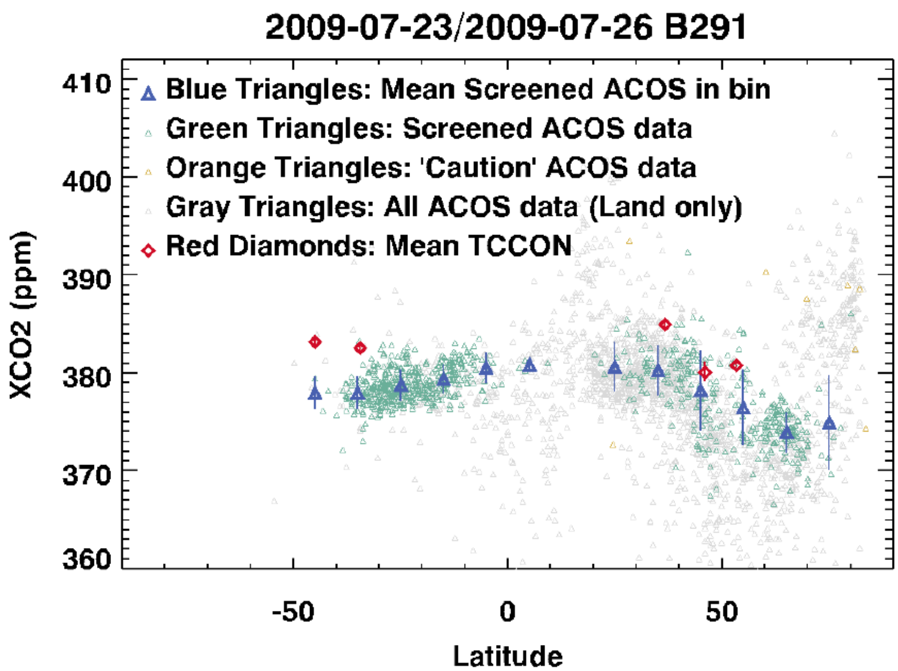

Figure 4-3. Comparison of ACOS column measurements with TCCON data for three days in July 2009. Comparisons like these will also be a standard output of the different software tests implemented during the ACOS task.

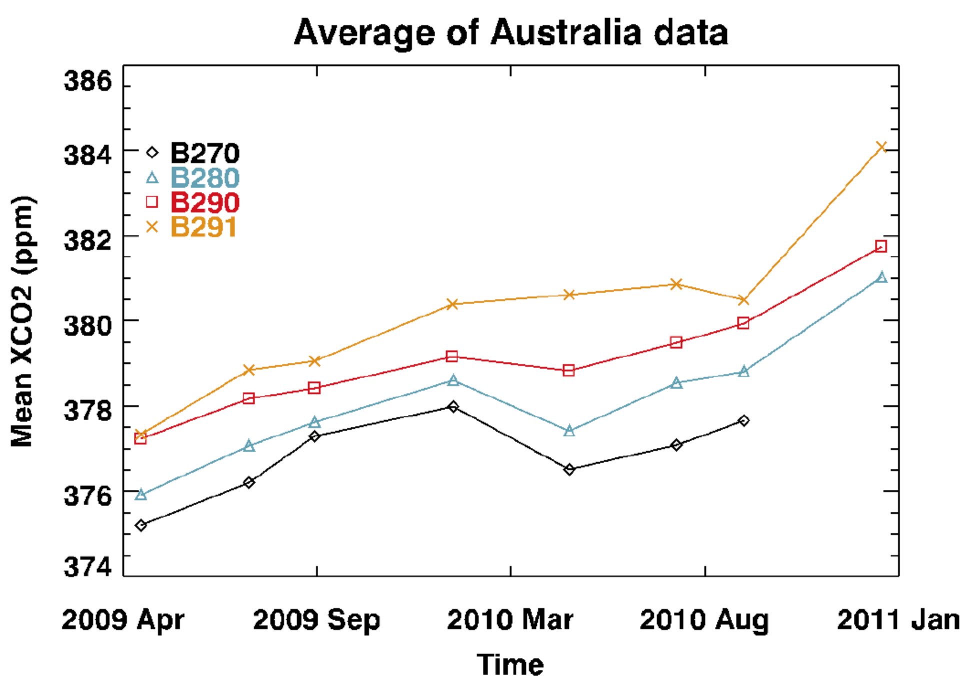

Figure 4-4. Time series of the mean X_{CO2} values and how they change per software release.

The particular quantities used to diagnose the OCO-2 retrievals will be different from those used in ACOS, but the work done on the ACOS data and results from the OCO-2 system test will allow us to define a set of key parameters prior to launch.

4.3.4 Science Acceptance Testing and Data Characterization

Once a new build of the OCO-2 retrieval software is ready to be tested, it will be run through a larger set of data to determine the quality of the data, begin testing strategies for screening the data and getting a better estimate of the bias. During the ACOS project this happened in two phases, "Science Acceptance Testing" and "Data Characterization".

Science acceptance testing is designed to test the data results over a significant, but still relatively small amount of data, on the order of two months (for ACOS testing these data were spread out over an 18 month period). Results from this data were used during ACOS to provide a determination of whether the software release was ready to go into production on the larger data set. The Validation team provided the metrics and plots for the larger Science team to evaluate and a consensus was obtained from the team to move forward, present the release to an OCO-2 Configuration Change Board (CCB) and the proceed with data production using the new retrieval software.

The final step of data testing is the Data Characterization phase, which uses a large percentage of the full data set (approximately one year of data). The metrics and plots are similar to the previous steps of testing. Examining the effects of atmospheric properties such as aerosols, clouds, humidity and temperature to provide insight into their effects on bias and data quality are a key component of this round of testing. There will be a large amount of data available to improve the data screening criteria and provide this information to the data users.

4.3.5 Algorithm Testing and Validation

Overall, the hierarchy of tests described above provides a guide to what will be done once OCO-2 begins operation in orbit. In the early stages of the project, there may not be time to perform a full data characterization. The regression, enhanced regression and science acceptance testing will definitely be part of the algorithm and validation processes for OCO-2. During the ACOS task, the Science team worked to determine the diagnostic fields (provided in the data products) required for doing a proper validation of the X_{CO2} product. The team also worked to include validation analyses within the algorithm testing, using comparisons to TCCON data to allow us to help quantify how changes in the code are affecting the retrieved data product.

5. Validation Plan Summary

The OCO-2 Validation Plan has been updated from the version developed for the OCO instrument; however the core strategies put in place in that document remain in place. The requirement to validate the space based measurements of X_{CO2} will be met by comparing OCO-2 data to ground based measurements from the TCCON network. The space based measurements will be tied to the NOAA ESRL (Earth Sciences Research Laboratory) standard by a chain of comparison and calibration studies linking OCO-2, TCCON, aircraft and surface in situ measurements. The TCCON network has matured significantly over the past 5 years and is the critical component for validating X_{CO2} from OCO-2.

The validation team will focus on understanding any bias observed between the OCO-2 and TCCON data through regression analyses as described in Wunch et al. [2011b]. These analyses will allow the validation team to estimate the effects of aerosols, air mass effects and other atmospheric properties on the observed bias between X_{CO2} observations. These validation analyses have been tested as a part of the ACOS task where data from the GOSAT TANSO-FTS instrument was processed through the OCO-2 Level 2 retrieval algorithm. The X_{CO2} product from ACOS was made available to the scientific community and the preliminary validation was described in Wunch et al. [2011b]. The ACOS task allowed for a rehearsal of the validation plan as spelled out in this document. In addition, the ACOS task has allowed for the development of a hierarchy of testing for the retrievals from the Level 2 algorithm. These tests provide a means for communication between the algorithm and validation teams, allowing the validation team to perform preliminary validation analyses and feed that information back to the algorithm team during the software development process. While not strictly a full science validation, this testing process has provided critical information on the effects of changes to the software code on the Level 2 products through comparisons to the TCCON data. These types of tests will be updated for use with OCO-2 data when it becomes available and provide the initial results toward a full science validation of the OCO-2 X_{CO2} product. This close interaction between algorithm updates and science data validation combined with the full analysis of TCCON and satellite data will allow for a thorough validation of the OCO-2 X_{CO2} product.

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7. Acronyms

ACOS	Atmospheric CO_2 Observations from Space
ARM	Atmospheric Radiation Monitoring
CAR	*Corrective Action Request*
CH_4	Methane
CO	Carbon Monoxide
CO_2	Carbon Dioxide
COBRA	CO2 Budget and Rectification Airborne
ESRL	Earth Sciences Research Laboratory
FOV	Field of View
FTS	Fourier Transform Spectrometer
GFIT	Algorithm developed at JPL for the analysis of solar absorption spectra.
GOSAT	Greenhouse Gases Observing Satellite
H_2O	Water
HCL	Hydrochloric acid
HIAPER	High-performance Instrumented Airborne Platform for Environmental Research
HIPPO	HIAPER Pole-To-Pole Observations
HITRAN	High Resolution Transmission
INTEX	Intercontinental Chemical Transport Experiment (US NASA)
IOC	In-Orbit Check-out
IR	Infrared
JAXA	Japan Aerospace Exploration Agency
JPL	Jet Propulsion Laboratory
km	kilometer
MOC	*Management of Change*
MoE	Ministry of the Environment (Japan)
MPS	Mission Planning System
NASA	National Aeronautics and Space Administration
NIR	Near Infrared
NOAA	National Oceanic and Atmospheric Administration
O_2	Oxygen

OCO	Orbiting Carbon Observatory
ppm	parts per million
RTS	Relative Time Sequences
SWIR	Shortwave Infrared
TANSO	Thermal And Near infrared Sensor for carbon Observation
TANSO-CAI	Thermal And Near infrared Sensor for carbon Observations - Cloud and Aerosol Imager
TCCON	Total Carbon Column Observing Network
TIR	Thermal Infrared
TWP-ICE	Tropical Warm Pool International Cloud Experiment (Australia)
UV-VIS-NIR	Ultra Violet – Visible - Near Infrared
WLEF	WLEF station tall-tower observation site in Wisconsin
WMO	World Meteorological Organization